Open Notebook Science: Chemical Rediscovery Survey

Library of Congress (FEDLINK)

Open Science Symposium

Jean-Claude Bradley

Associate Professor of Chemistry
Drexel University

November 12, 2013

Top 5 questions in chemistry according to Scientific American

(Nov 5, 2013)

1. Can we unravel the puzzle of life's origins?
2. Can we ever beat photosynthesis?
3. How do we make chemistry environmentally friendly?
4. Can we design the perfect drug?
5. How do we sell chemistry to the public?

The current paradigm of doing and sharing science in chemistry

1. Design experiments based on established or potentially new theories.
2. Execute and record experimental outcomes in private notebooks.
3. When a sufficient narrative emerges selective experimental data are combined to publish, with a limited amount of "supplementary supporting data"

What kind of (chemical) worldview has this approach created?

1. Selective bias towards which experiment are even attempted.

2. Overconfidence in our understanding since deviant or ambiguous results are rarely reported.

Filling in the blind spots with the **Chemical Rediscovery Survey**

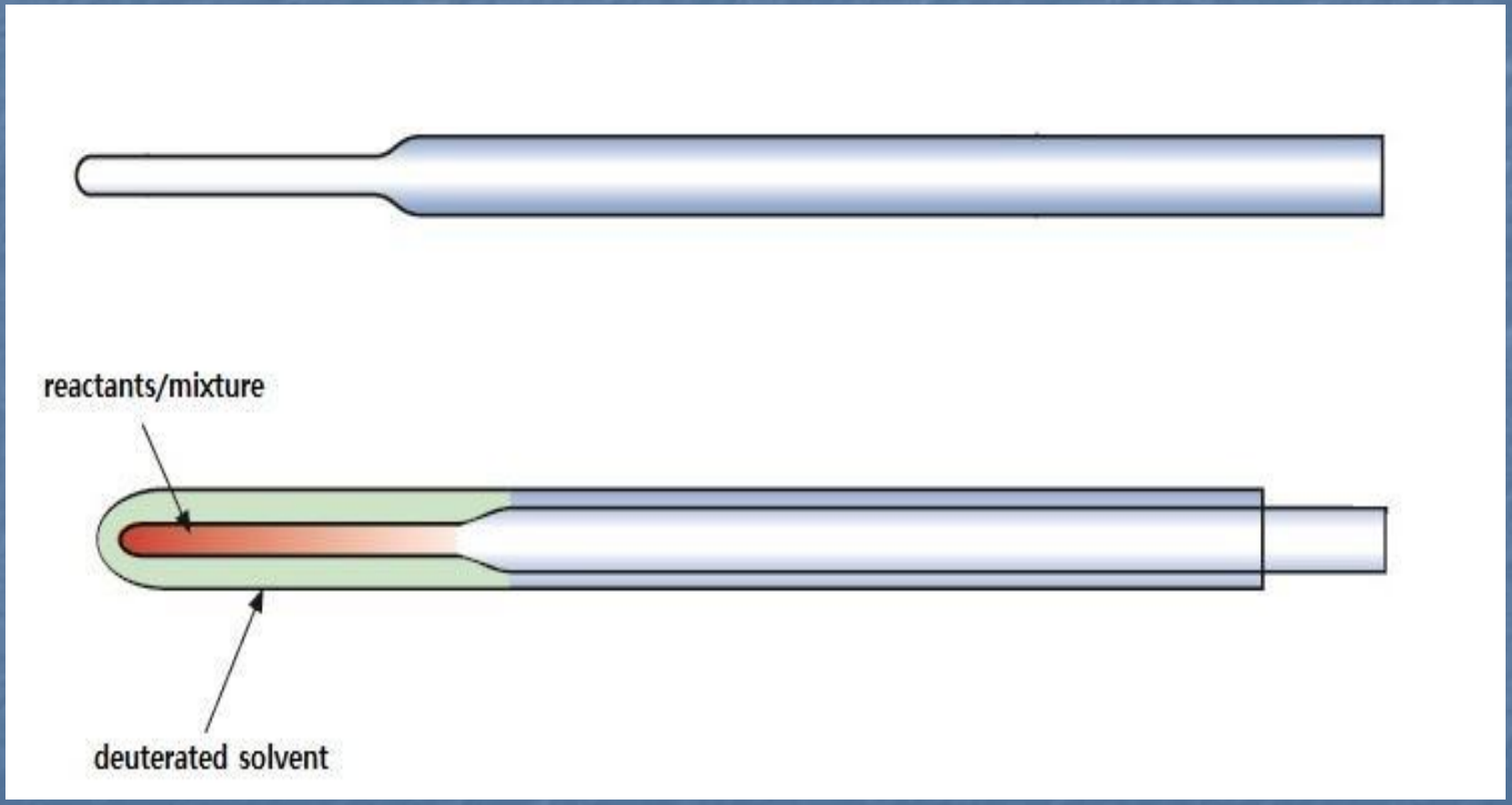
(chemrs.wikispaces.com)

1. Randomize the mixture of chemicals with certain criteria*
2. Identify "what happens" after convenient* periods of time.
3. Follow up on unexpected behavior with the traditional scientific method.
4. Openly share the entire process, including all raw data and preliminary hypotheses and discoveries as it happens.

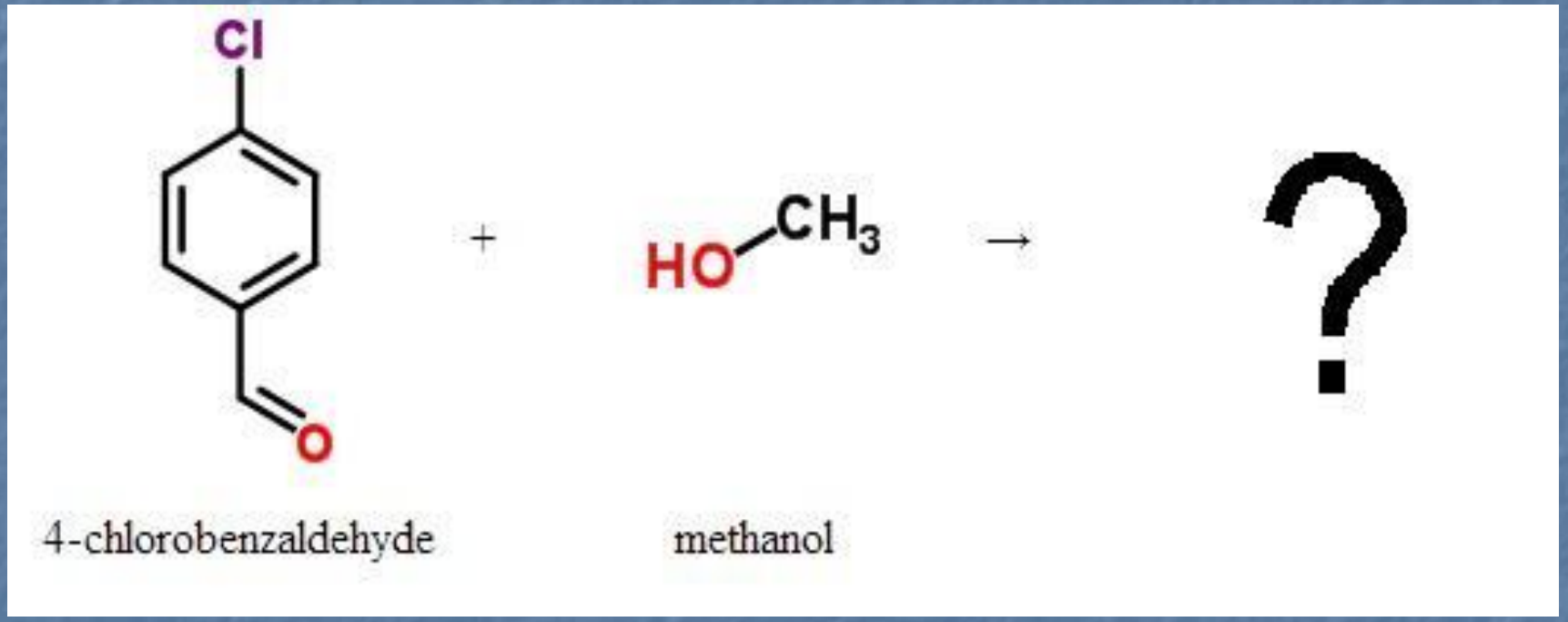
The current CRS criteria

1. Only small common cheap organic compounds
2. Only select relatively "Green" compounds
3. Avoid excessively unpleasant compounds (stench!)

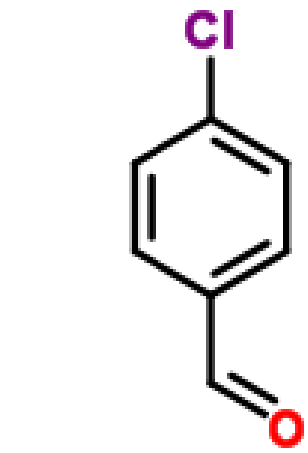
Co-axial NMR tubes are used to isolate the reaction from the deuterated solvent



An example of a Chemical Rediscovery Survey experiment



The overall reaction is easily identified by NMR

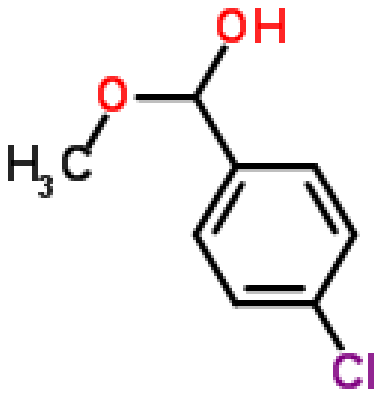


4-chlorobenzaldehyde

+

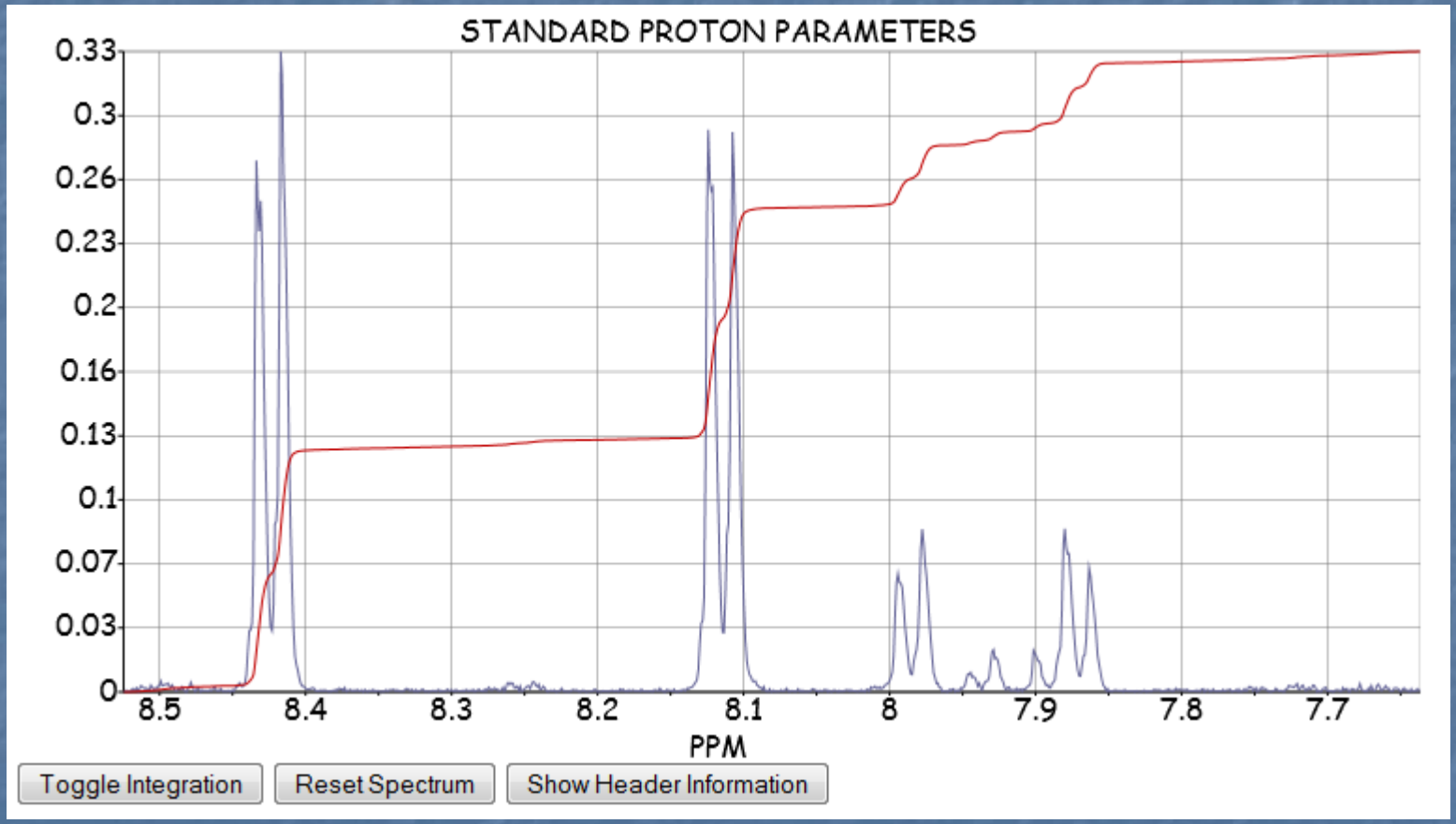
methanol

→

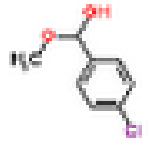


4-chlorobenzaldehyde methanol hemiacetal

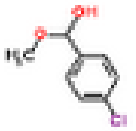
Raw NMR data is provided for open analysis



The experiment is represented in a machine readable matrix: mole fractions

ARRAYID	EXP	mole fraction sum	4-chlorobenzaldehyd	methanol	4-chlorobenzaldehyd methanol hemiacetal
			mole fraction	mole fraction	mole fraction
Image					
CSID			21106019	864	26559511
CS link			http://chemspider.c	http://chemspider.c	http://chemspider.c
9	2	1	0.013326475345 07	0.983765105742 23	0.002908418912 69

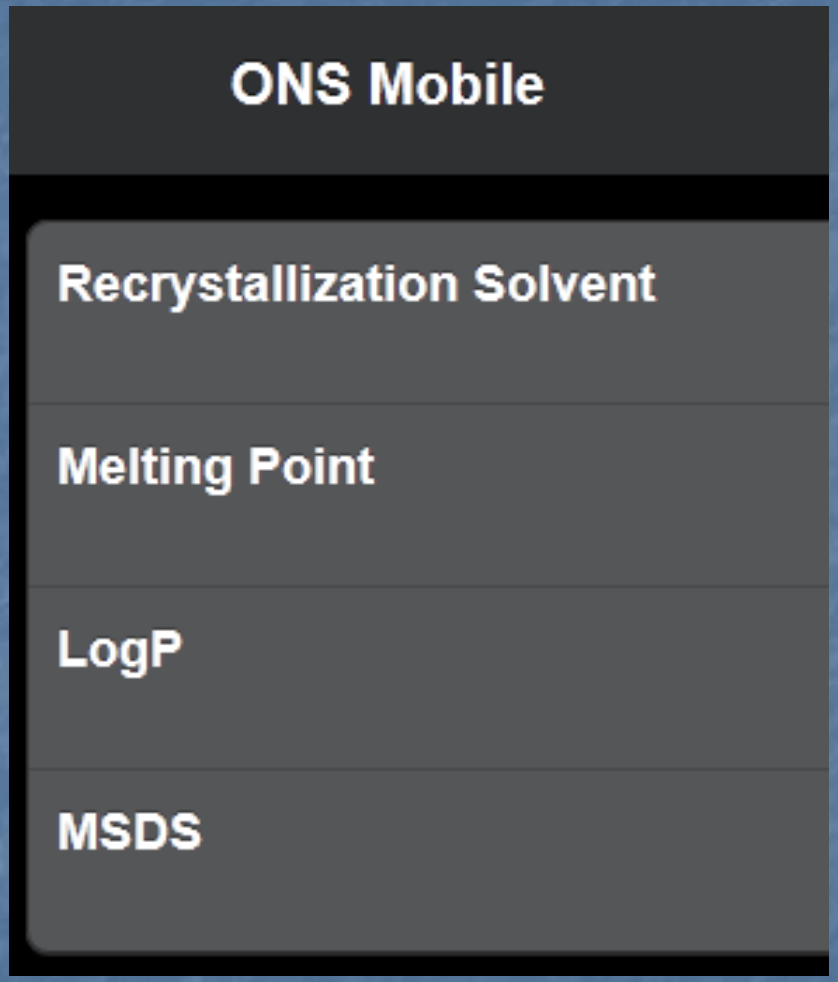
All assignable NMR peaks are also archived for machine readability

4-chlorobenzaldehyd methanol hemiacetal	4-chlorobenzaldehyde methanol hemiacetal	4-chlorobenzaldehyd methanol hemiacetal	4-chlorobenzaldehyd methanol hemiacetal	4-chlorobenzaldehyd methanol hemiacetal	4
HNMR Ar	HNMR Ar	HNMR OH	HNMR Bn	HNMR CH3	H
					
26559511	26559511	26559511	26559511	26559511	
http://chemspider.c	http://chemspider.cor	http://chemspider.c	http://chemspider.c	http://chemspider.c	
8.005(2H, d, J=8.25Hz)	7.889(2H, d, J=8.25Hz)	?	6.07(1H, s)	?	

NMR requires a homogeneous solution for proper measurement

However once an interesting reaction has been observed to occur slowly at 25C and low concentration, preparative scale-up conditions can be estimated (i.e. reaction rate doubles about every 10C)

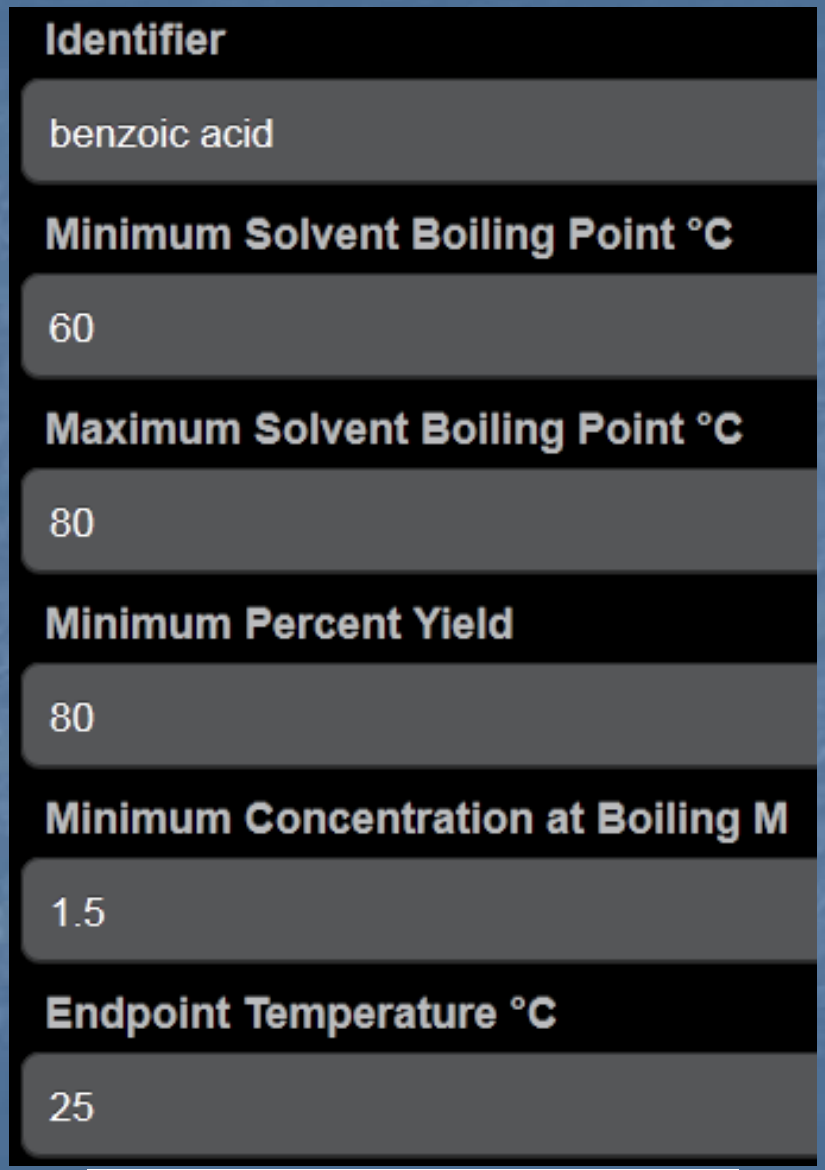
The Recrystallization App (Open)



http://xtalapp.wikispaces.com

(Andrew Lang)

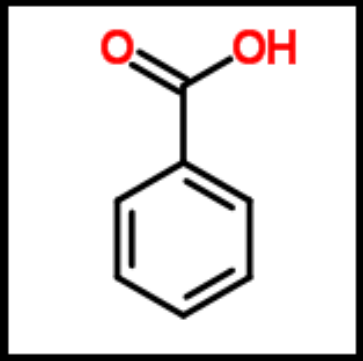
What are good solvents to recrystallize benzoic acid?



http://xtalapp.wikispaces.com

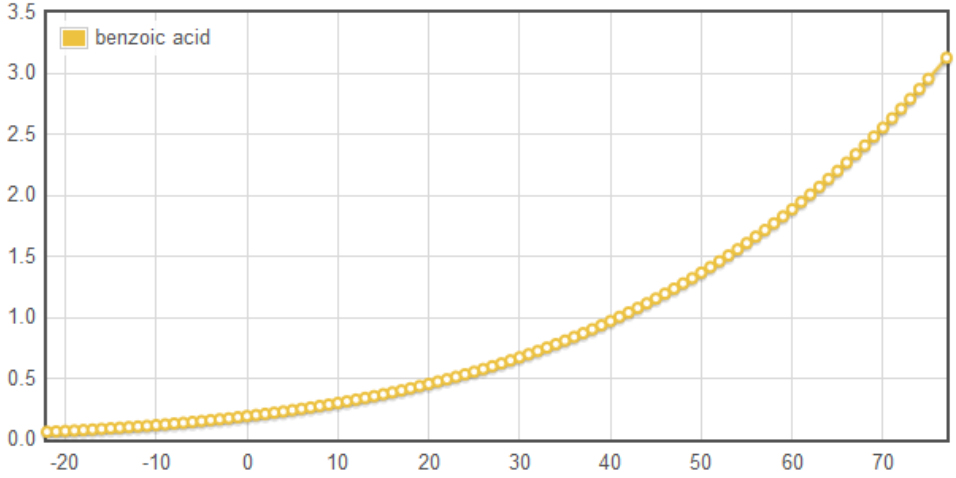
(Andrew Lang)

Click on the solvent to see temp curve (Open)

benzoic acid	
	
1-chlorobutane	94%
ethanol/water(30:70)vol	93%
ethanol/water(40:60)vol	85%
carbon tetrachloride	82%

Solubility (M) in carbon tetrachloride from -22.4C (mp) to 76C (bp)

	benzoic acid
miscible point	9.8M
melting point	122.42C



http://xtalapp.wikispaces.com

(Andrew Lang)

The role of Openness in rethinking how to tackle the "big chemistry questions"

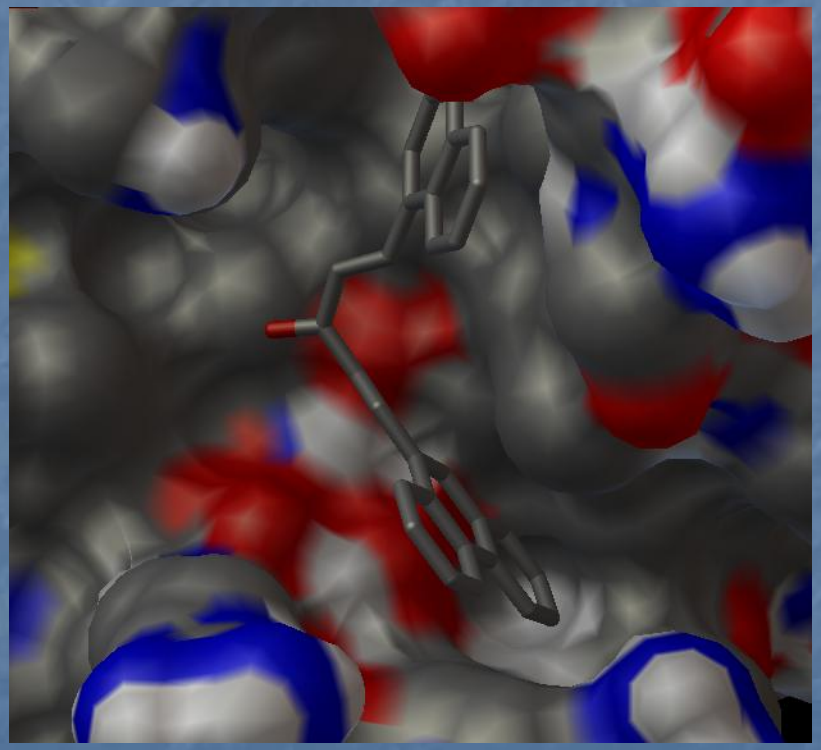
Q3. How do we make chemistry environmentally friendly?

By limiting ourselves to relatively Green compounds and by sharing all data in real time we are much more likely to find Green reactions from the CRS project and encourage others to benefit.

This would reduce student exposure in teaching labs and lower costs for waste disposal

Q4. Can we design the perfect drug?

We can try to do Open Drug Discovery – we have found active lead compounds against malaria for example and working on Taxol analogs



http://usefulchem.wikispaces.com/D-EXP022

(Andrew Lang)

Q5. How do we sell chemistry to the public?

We are approaching 1000 queries a day for specific solubility and melting point data. Some originate from academia and industry but many from high schools and the general public.

By concentrating on "Green" non toxic and readily available compounds and by providing Open resources to encourage their curiosity the public will become more engaged and understand the importance of chemistry.

Contributing to Science while Teaching it: Chemical Information Retrieval Class

Chemical Information Retrieval

Drexel University Course CHEM 367-767

Fall 2012

Instructor: Jean-Claude Bradley bradlejc AT drexel.edu

Location: CAT 268

Times: Fridays 16:00-18:50

cheminfo2012.wikispaces.com

Syllabus
resources
assignments
cheminformatics guide
cheminfo sheet 2012
full cheminfo sheet (read-only)
web services
FAQ2009
FAQ2010
FAQ2011

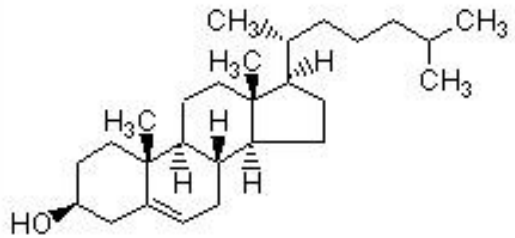
Chemical Information Validation Sheet 2012

chemical name	property	source value	source units	common value	common units	link	data source type	image	notes	status
cholesterol	melting point	148-150	C	422.15	K	http://www.tciche	Chemical Vendor	http://cheminfo2012.wikisp /file/view /Cholesterol+Tokyo+Chemi /371712938 /Cholesterol%20Tokyo%20		done
cholesterol	optical rotation	-36	degrees	-36	degrees	http://www.alfa.c	Chemical Vendor	http://cheminfo2012.wikisp /file/view /Cholesterol+Alfa+Aesar.jp /371713216 /Cholesterol%20Alfa%20Ae	C=2, Dioxane	done
cholesterol	boiling point	360	C	633.15	K	http://appft1.uspt	Patent Application	http://cheminfo2012.wikisp /file/view /Cholesterol+Patent.jpg /371716670 /Cholesterol%20Patent.jpg		done
cholesterol	solubility (aqueous)	4.7	uM	0.0000047	M	http://www.pnas. /content /70/8/2313.full.pd	peer reviewed journal	http://cheminfo2012.wikisp /file/view /Cholesterol+Solubility+Se association+of+cholesterol /372022946 /Cholesterol%20Solubility% association%20of%20chole	25C	done

Each entry validated with an image

Cholesterol
(CAS Number : 57-88-5)

Structure



Specification

Purity(GC)	min. 95.0 %
Melting point	148.0 to 150.0 deg-C
Specific rotation [a]25/D	-34.0 to -39.5 deg(C=2, Dioxane)
Solubility in hot EtOH	very faint turbidity

Data of Reference

mp	149°C
[a]20D	-37° (C=2,Dioxane)

Alfa Aesar donates melting points to the public

Alfa Aesar®
A Johnson Matthey Company

DSSTK	DSDESC	DSPURE	DCMELT
H26903	(-)-1,4-Di-O-tosyl-2,3-O-isopropylidene-L-threitol	98%	90°
B24134	(-)-2,3-O-Isopropylidene-D-threitol	98%	45-49°
L04759	(-)-alpha-Pinene	98%, cont. variab	-64°
A12684	(-)-Borneol	98%	205-208°
A18040	(-)-Camphene	tech. 80%	ca 35°
A18796	(-)-Cinchonidine	99% (total base),	201-206°
A16180	(-)-Dibenzoyl-L-tartaric acid monohydrate	98+%	90-92°
A16181	(-)-Dibenzoyl-L-tartaric acid, anhydrous	99%	154-156°
A17992	(-)-Diethyl D-tartrate	99%	17°
B21029	(-)-DIOP	98%	88-90°
L15151	(-)-Fenchone	98+%	3-5°
L18485	(-)-Lupinine	97%	62-65°
41570	(-)-N-Methylephedrine	98+%	86°-88°
L04848	(-)-Shikimic acid	98%	184-188°
B23090	(+)-2,3-O-Isopropylidene-L-threitol	98%	45-49°
A11542	(+)-5-Iodo-2'-deoxyuridine	98%	ca 190° dec.

http://usefulchem.blogspot.com/2011/02/alfa-aesar-melting-point-data-now.html

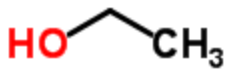
Outliers for ethanol: Alfa Aesar and Oxford MSDS

name	mp °C	source	SMILES	
ethanol[1]	-130.00	Alfa Aesar	CCO	use
ethanol	-114.00	American Petroleum Institute	CCO	do not use
Ethanol[2]	-144.00	academic website	CCO	use
Ethanol	-114.10	DrugBank	CCO	do not use
ethanol	-114.10	PHYSPROP	CCO	do not use
ethanol	-114.14	commercial database	CCO	cheminfo
ethanol	-114.40	commercial database	CCO	cheminfo
ethanol	-114.00	academic website	CCO	cheminfo
ethanol	-114.00	chemical vendor	CCO	cheminfo
ethanol	-114.30	crowdsourced database	CCO	cheminfo

compound: ethanol - melting point: -114.13 °C

Entries highlighted in red are not used in calculating the average value:

1. confirmed error with source JCB
2. clearly out of range JCB



http://usefulchem.blogspot.com/2011/03/validating-melting-point-data-from-alfa.html

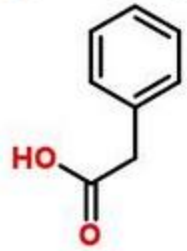
Outliers

MDPI dataset

OPEN Notebook Science

name	mp °C	source	SMILES
phenylacetic acid	77.50	Alfa Aesar	c1ccc(cc1)CC(=O)O
PhenylessigsÃ□ure	150.00	peer reviewed journal	O=C(O)Cc1ccccc1
phenylacetic acid	76.70	government database	O=C(O)Cc1ccccc1
phenylacetic acid	77.00	commercial database	O=C(O)Cc1ccccc1
phenylacetic acid	77.50	commercial database	O=C(O)Cc1ccccc1

The average melting point of phenylacetic acid is 91.74 °C

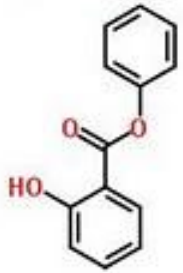


EPI (donated all data to public also)

OPEN Notebook Science

name	mp °C	source	SMILES
phenyl salicylate	43.00	Alfa Aesar	c1ccc(cc1)OC(=O)c2ccccc2O
phenyl salicylate	130.50	government database	O=C(Oc1ccccc1)c2ccccc2O
phenyl salicylate	42.00	chemical vendor	O=C(Oc1ccccc1)c2ccccc2O

The average melting point of phenyl salicylate is 71.83 °C



http://usefulchem.blogspot.com/2011/03/validating-melting-point-data-from-alfa.html

http://usefulchem.blogspot.com/2011/05/more-open-melting-points-from-epi-and.html

Open Melting Point Datasets
Currently 20,000 compounds with Open MPs

ONSMP000: (ONSCwiki) 15591 full raw entries from Alfa Aesar containing duplicates and non numerical values
ONSMP001: (ORU) 12986 measurements as simple numeric values converted from mp ranges and other entries with non-numeric characters from Alfa Aesar (ONSMP000).
ONSMP002: (ORU) 8739 measurements derived from ONSMP001 with redundancies, salts, inorganics and organometallics removed. Silicon, phosphorus and boron containing organic compounds were retained. SMILES, CSIDs and links to the Alfa Aesar catalog are included.
ONSMP003: (ORU) 4450 measurements from Karthikeyan 2005. Includes SMILES and many descriptors.
ONSMP004: (ORU) 4084 measurements derived from ONSMP003 - includes compound names and CSIDs - excludes SMILES that did not properly render with OpenEye. 48 compounds were missing from ONSMP004 that were in ONSMP003 - these have been recovered but they do not have associated names or CSIDs: ONSMP004a
ONSMP005: (ORU) 277 measurements from Bergstrom 2003. Drug molecules separated as training and validation sheets. SMILES provided.
ONSMP006 (ORU) 277 measurements derived from ONSMP005 compiled into one sheet and both SMILES and CSIDs provided.
ONSMP007 (pending) curated Karthikeyan dataset ONS004 further curated by removal of all duplicate entries (with very different melting points)
ONSMP008 (ONSCwiki) 33 Duplicates (66 measurements) with a difference with more than 10C from the Karthikeyan dataset ONSMP003
ONSMP009 (ONSCwiki) 311 SMILES which could not be rendered correctly on ChemSketch from Karthikeyan dataset ONSMP003
ONSMP010 (ONSCwiki) 150 SMILES consisting of all EPI melting point data (via ChemSpider) from a 2011-03-04 snapshot of Cheminfo Validation sheet. 106 of these have at least one MP from another source. 10 of the 106 show a difference of at least 5C between the EPI and the other sources.
ONSMP011 (ONSCwiki) 335 measurements. A snapshot taken 2011-02-20 of the crowdsourced melting point data in the ChemInfo Validation Sheet.
ONSMP012 (ONSCwiki) 1286 measurements removed from the union of ONSMP002, ONSMP003, ONSMP006, and ONSMP011. Data were removed because they were either salts, had a large discrepancy in measurements (greater then 10C), were suspected erroneous measurements, were unneeded duplicates, or failed to produce CDK desscriptors, see meltingpointmodel001.
ONSMP013 (ORU) 12634 highly curated (see ONSMP012 above) unique melting point measurements with CDK descriptor values based upon the union of ONSMP002, ONSMP003, ONSMP006, and ONSMP011.

http://onschallenge.wikispaces.com/Open+Melting+Point+Datasets

What is the melting point of 4-benzyltoluene?

American Petroleum Institute	5 C
PHYSPROP	-30 C
PHYSPROP	125 C
peer reviewed journal (2008)	97.5 C
government database	-30 C
government database	4.58 C

Open Lab Notebook page measuring the melting point of 4-benzyltoluene

Exp266 Edit This Page | page | discussion | history | notify me

Researcher

Evan Curtin and Jean-Claude Bradley

Objective

To determine the melting point of 4-benzyltoluene to clarify discrepancies in melting point data.

Procedure

The sample of a few grams in a sealed bottle or tube was frozen then allowed to warm back up and an attempt to measure the melting point from the appearance of the sample was made.

Conclusion

After 2 days in the freezer the sample remains unfrozen at -15C. However, after 16 days the sample was found frozen at -14C Immersion in an ice bath and very slow heating over a few hours revealed that complete melting happened at 4-6 C.

Log

2011-06-03

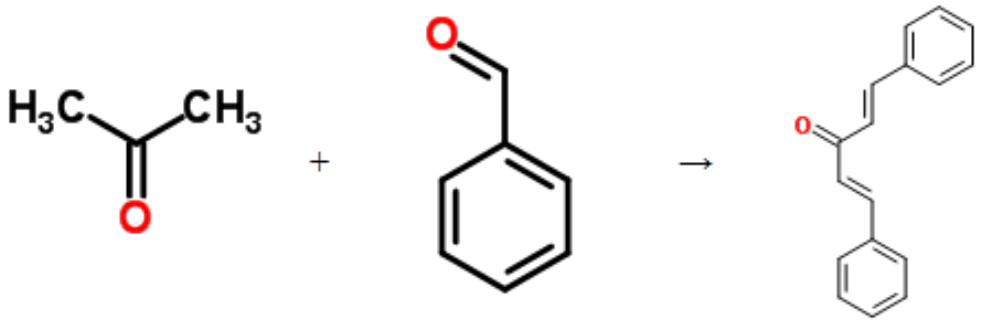
11:20 - Removed 4-benzyltoluene container from package, observed that it is a liquid at room temperature (25C) - pic 1
11:31 - Wrapped in parafilm, put in 0C bath. - pic 2
11:34 - No change in viscosity of the sample
11:52 - Moved sample to an acetone bath, slowly added dry ice. Sample was not frozen at -5C (bath temperature)
12:00 - unclear when sample froze but after letting heat up to -18C sample still frozen - pic 3

http://usefulchem.wikispaces.com/Exp266

An example of a failed experiment in an Open Notebook with useful information

Reaction ID ONSEXP269

Researcher	Matthew McBride
Reaction Type	aldol condensation
Solvent	ethanol/water (1:6)vol
Limiting Reactant	0.43 M
Precipitate	No
Comments	Used KOH as base catalyst; benzaldehyde did not fully dissolve
Reference	http://onschallenge.wikispaces.com/EXP269
Solvent Selection	Optimal Solvent Prediction



acetone benzaldehyde dibenzalacetone

A failed experiment reveals the importance of aldehyde solubility

EXP269

Researcher

Matthew McBride

Conclusion

The reaction likely failed because the benzaldehyde could not be fully solubilized with the amount of ethanol used relative to water. This synthesis was successfully completed in EXP279 with 1:1 ethanol/water, compared to only 1:6 ethanol/water used in this experiment.

Log

2012-03-12

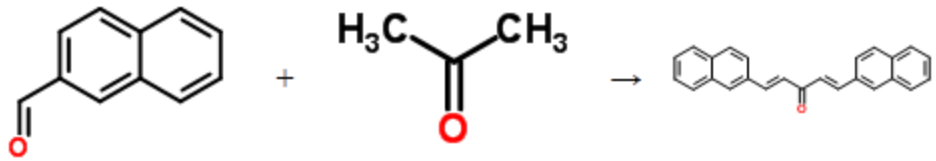
12:25 Added 28g of KOH to each of 500mL Erlenmeyer flasks.
12:33 Added 30mL of ethanol to each flask.
12:46 Added an additional 28g of KOH to flask 2 so that the flask had a total of 56g of KOH.
12:53 Added 180mL of distilled water to each flask.
13:11 Added 10mL of benzaldehyde to each flask. This value is approximate because there was difficulty with the needle used to remove the benzaldehyde from the glass bottle.
13:19 Placed flask 2 on the stirrer and the solution was observed to turn an orange color.
13:22 Place flask 1 on an old stir plate that did not stir the solution very well.
13:41 Removed beaker two from the stir plate and placed on ice. The solution was observed to separate into two layers. A thin top layer that looked oily and was of a orange color. The bottom layer was of a pale yellow color. No crystals were observed to form.
14:00 No crystals were visible in either flask and it was determined that the reaction had not been completed.

http://onschallenge.wikispaces.com/EXP269

Information from the literature on the target synthesis

Reaction ID Ref005

Researcher	Seifert96
Reaction Type	aldol condensation
Solvent	-
Limiting Reactant	- M
Precipitate	Yes
Yield	- %
Comments	Refers to Organic Syntheses Paper. Provides no additional details
Reference	http://dx.doi.org/10.1016/0040-4020(96)00788-0



Open Notebook Science

From Wikipedia, the free encyclopedia

Open Notebook Science is the practice of making the entire primary record of a research project publicly available online as it is recorded. This involves placing the personal, or laboratory, notebook of the researcher online along with all raw and processed data, and any associated material, as this material is generated. The

References

1. ^ [a] [b] Goetz, T. Freeing the Dark Data of Failed Scientific Experiments Wired Magazine, Sept.25, 2007.
2. ^ Sanderson, K (September 2008). "Data on display". *Nature*. doi:10.1038/455273a.
3. ^ Singh, S. (April 2008). "Data on display". *Cell*. doi:10.1016/j.cell.2008.04.003.
4. ^ Lloyd, R. Era of Scientific Secrecy Near End Live Science, Sept 2, 2008.
5. ^ Williams, A. J. Internet-based tools for communication and collaboration in chemistry Drug Discovery Today, vol 13, p. 502 (2008).
6. ^ Everts, S. Open Source Science, Chemical & Engineering News, July 2006, 84 (30) p. 34.

Motivation: Faster Science, Better Science

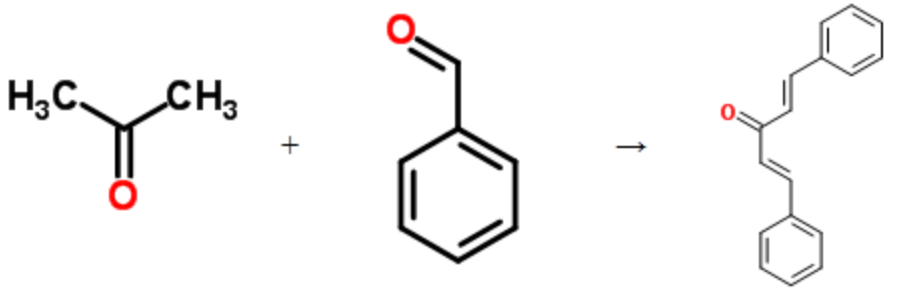
There are NO FACTS,
only measurements embedded
within assumptions

Open Notebook Science maintains
the integrity of data provenance by
making assumptions explicit

An example of a successful experiment in an Open Notebook that was used to improve the teaching lab manual

Reaction ID UCEXP284

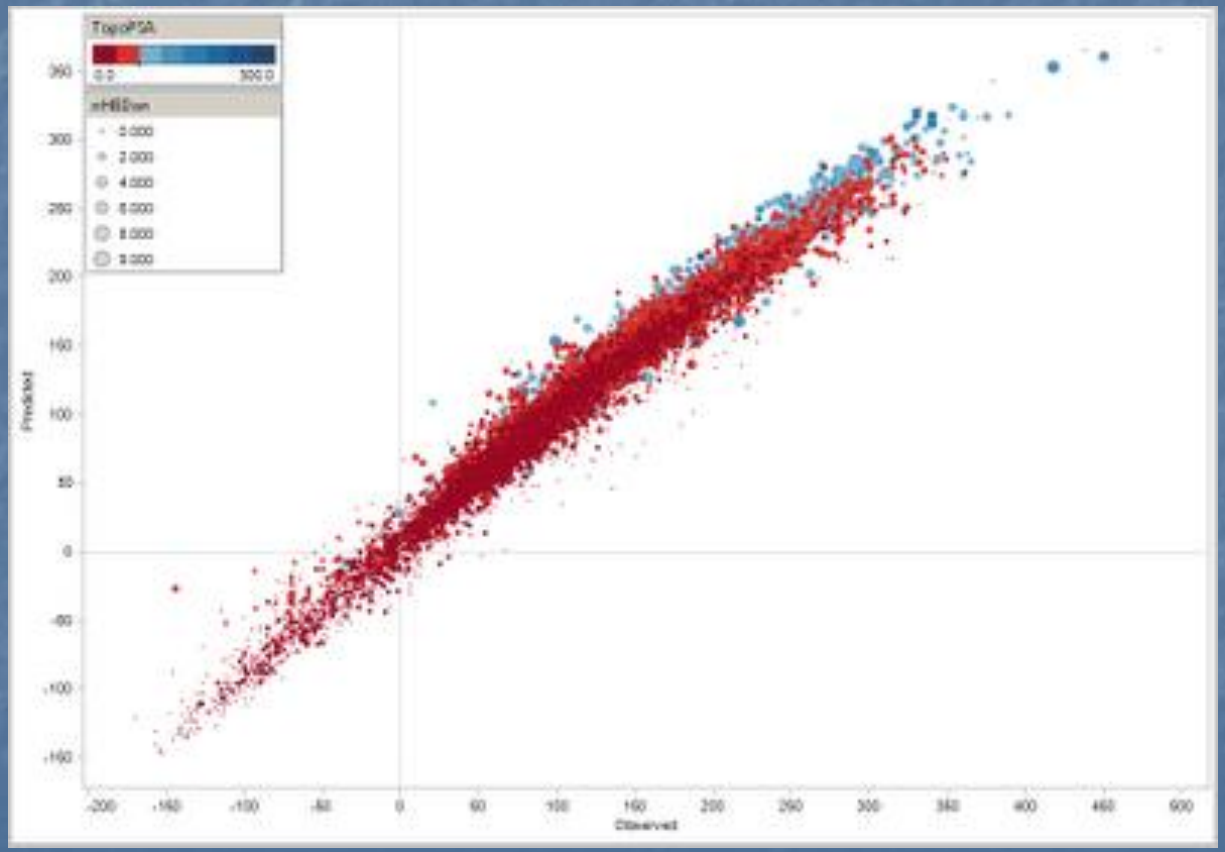
Researcher	Matthew McBride
Reaction Type	aldol condensation
Solvent	ethanol/water (1:1)vol
Limiting Reactant	0.17 M
Precipitate	Yes
Yield	87 %
Comments	NaOH catalyst (1.7 eq to acetone); 2.7 eq benzaldehyde to acetone; 35 min rt then flitered; no re-crystallization required
Reference	http://usefulchem.wikispaces.com/EXP284
Solvent Selection	Optimal Solvent Prediction



acetone benzaldehyde dibenzalacetone

Open Random Forest modeling of Open Melting Point data using CDK descriptors (Andrew Lang)

R2 = 0.78, TPSA and nHdon most important



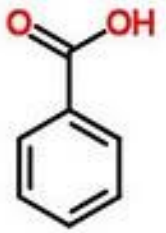
http://usefulchem.blogspot.com/2011/03/open-modeling-of-melting-point-data.html

Melting point prediction service

OPEN Notebook Science

name	mp °C	source	SMILES
benzoic acid	123.00	Alfa Aesar	c1ccc(cc1)C(=O)O
benzoic acid	122.00	peer reviewed journal (sup. data)	OC(=O)c1ccccc1
Benzoic Acid	122.00	peer reviewed journal (sup. data)	O=C(O)c1ccccc1
benzoic acid	122.40	government database	c1ccc(cc1)C(=O)O
benzoic acid	122.00	peer reviewed journal	c1ccc(cc1)C(=O)O
benzoic acid	122.00	peer reviewed journal	c1ccc(cc1)C(=O)O
benzoic acid	123.00	chemical vendor	c1ccc(cc1)C(=O)O
benzoic acid	122.35	commercial database	c1ccc(cc1)C(=O)O
benzoic acid	122.40	commercial database	c1ccc(cc1)C(=O)O

The average melting point of benzoic acid is 122.35 °C



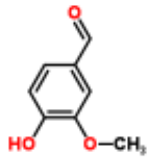
Predicted melting point °C.
107.91

http://usefulchem.blogspot.com/2011/03/open-modeling-of-melting-point-data.html

Web services for summary data

OPEN NOTEBOOK SCIENCE CHALLENGE

These results are from the Open Notebook Science Solubility Challenge as of January 15, 2011
A compilation of the results in book form can be obtained from Nature Precedings



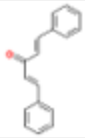
Solubility of vanillin in organic solvents.
Total Number of Results: 17
Total Number of Solvents: 9

	Solvent	Ave. (M)	Hits	SD	Link to Detailed Results
1.	**1,2-dichloroethane**	**1.175**	1	0.000	Solubility of vanillin in 1,2-dichloroethane is 1.175 M
2.	**1-propanol**	**1.820**	1	0.000	Solubility of vanillin in 1-propanol is 1.820 M
3.	**THF**	**3.594**	2	0.419	Solubility of vanillin in THF is 3.594 M
4.	**acetonitrile**	**2.360**	2	0.028	Solubility of vanillin in acetonitrile is 2.360 M
5.	**butanone**	**2.138**	1	0.000	Solubility of vanillin in butanone is 2.138 M
6.	**ethanol**	**2.470**	5	0.152	Solubility of vanillin in ethanol is 2.470 M
7.	**methanol**	**4.160**	3	0.026	Solubility of vanillin in methanol is 4.160 M
8.	**toluene**	**0.302**	1	0.000	Solubility of vanillin in toluene is 0.302 M
9.	**water**	**0.070**	1	0.000	Solubility of vanillin in water is 0.070 M

Permalink: http://old.oru.edu/cccda/sl/solubility/allsolvents.php?solute=vanillin

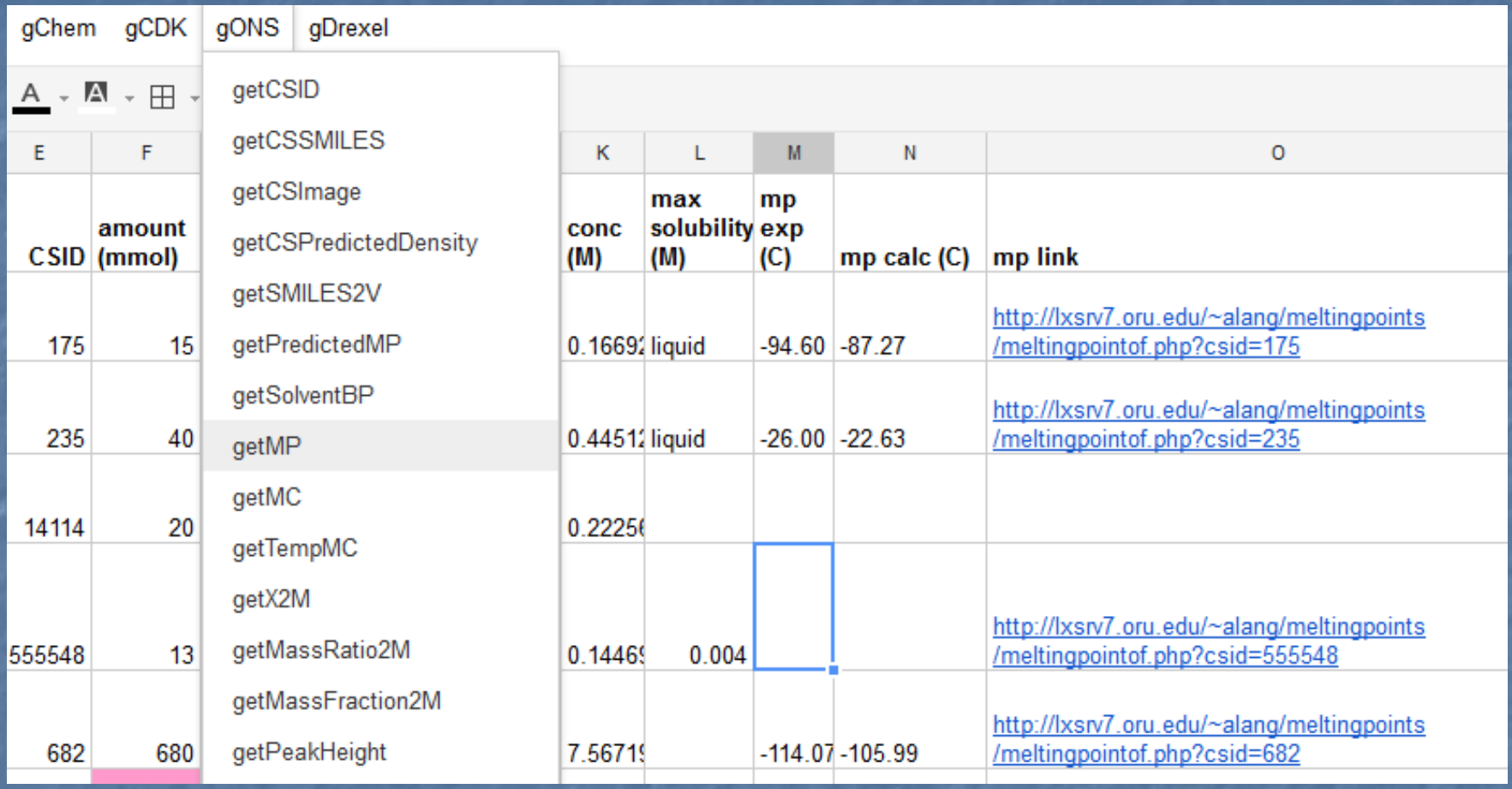
(Andrew Lang)

Using a Google Spreadsheet as a "dashboard interface" for reaction planning and analysis

Type	image	Name	SMILES	CSID	amount (mmol)	MW	amount (g)	density (g/ml)	volume (ml)	conc (M)	max solubility (M)	mp exp (C)	mp calc (C)
reactant		acetone	CC(=O)C	175	15	58.0418	0.87062	0.773	1.1262	0.1669	liquid	-94.60	-87.27
reactant		benzaldehyde	C(C1=CC=CC=C1)=	235	40	106.041	4.24167	1.05	4.0396	0.4451	liquid	-26.00	-22.63
reactant		sodium hydroxide	[OH-].[Na+]	14114	20	39.9925	0.79985	1	0.7998	0.2225			
product		trans-dibenzalaceto	C(C1=CC=CC=C1)=\C2=CC=CC=C2	555548	13	234.104	3.044	1.1	2.7672	0.1446	0.004		
solvent		ethanol	C(C)O	682	680	46.0418	31.3084	0.78	40.139	7.5671		-114.07	-105.99
solvent		water	O	937	2,250	18.0105	40.5237	0.999	40.564	25.038		0.00	-83.55
				yield (%)	86.7			total	89.861				

http://usefulchem.wikispaces.com/EXP284

Calling Google App Scripts



E	F	K	L	M	N	O
CSID	**amount (mmol)**	**conc (M)**	**max solubility (M)**	**mp exp (C)**	**mp calc (C)**	**mp link**
175	15	0.1669	liquid	-94.60	-87.27	http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=175
235	40	0.4451	liquid	-26.00	-22.63	http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=235
14114	20	0.2225				
555548	13	0.1446	0.004			http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=555548
682	680	7.5671		-114.07	-105.99	http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=682

http://onswebservices.wikispaces.com/GoogleAppsScripts

Calling Google App Scripts

gChem gCDK gONS gDrexel All changes saved

E	F	G	H	I	J	K	L	M	N	O
CSID	amount (mmol)	MW	amount (g)	density (g/ml)	volum (ml)	conc (M)	max solubility (M)	mp exp (C)	mp calc (C)	mp link
175	15	58.04186	0.87062	0.773	1.1262	0.16692	liquid	-94.60	-87.27	http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=175
235	40	106.0418	4.24167	1.05	4.0396	0.44512	liquid	-26.00	-22.63	http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=235
14114	20	39.99250	0.79985	1	0.7998	0.22256				
555548	13	234.1044	3.044	1.1	2.7672	0.14469	0.004	113.00		http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=555548
682	680	46.04186	31.3084	0.78	40.139	7.56719		-114.07	-105.99	http://lxsrv7.oru.edu/~alang/meltingpoints/meltingpointof.php?csid=682

http://onswebservices.wikispaces.com/GoogleAppsScripts

(Andrew Lang and Rich Apodaca)

Google Apps Scripts web services

http://onswebservices.wikispaces.com/GoogleAppsScripts

Google Apps Scripts for chemistry

Contributors

Andrew Lang, Rich Apodaca and Jean-Claude Bradley

Documentation

1. Rapid analysis of melting point trends and models using Google Apps Scripts (July 19, 2011 Jean-Claude Bradley) (link)
2. Practical Tips on using Google Apps Scripts for Chemistry Applications (July 14, 2011 Jean-Claude Bradley) (link)
3. gChem: Access Predicted and Calculated Chemical Substance Properties in Google Spreadsheets (July 13, 2011 Rich Apodaca) (link)
4. Google Apps Scripts for an intuitive interface to organic chemistry Open Notebooks (June 18, 2011 Jean-Claude Bradley) (link)
5. gChem: Convert Names and CAS Numbers to Chemical Structures in Google Spreadsheets (May 31, 2011 Rich Apodaca) (link)

Templates

Please do not edit this sheet - make a copy first. All of the Google Apps Script will be copied automatically. When the sheet opens the following three menu options should appear. If the three menu options do not appear hit the refresh button on your browser and wait a few seconds.

File Edit View Insert Format Data Tools Help gChem gCDK gONS

Reaction Planning Template 1 (based on an imine formation reaction UC-EXP269)
Melting point trend and modeling analysis (description)
Drexel library scripts (Is a compound in the CRC Handbook ?, Get article title from DOI and if it is in the library e-journal catalog)

Script details

GoogleAppsScripts summary sheet (Details about valid inputs and outputs, creator, type, status and descriptions)

Conclusions

More openness in chemistry can make science more efficient and address many of the key current questions challenging chemistry community

Provide interfaces that make sense to the end users:
Open Data, Open Models and Open Source Software to modelers
Apps (smartphones, Google App Scripts, etc.) for chemists at the bench

Acknowledgements

Andrew Lang (code, modeling)
Bill Acree (modeling, solubility data contribution)
Antony Williams (ChemSpider services, mp data curation)
Matthew McBride and Rida Atif (recrystallization and synthesis)
Kayla Gogarty, Cuepil Choi, Matthew McBride (CRS)